

Spring 2020 Colloquium

Department of Physics & Astronomy, TAMU-Commerce

Feb 27, Thursday, 4-5 PM in Science Building 127

(coffee and cookies will be served at 3:50 PM)

Computational condensed matter physics

**First-principles and multiscale simulations of electrified interfaces:
screening of two-dimensional materials for catalytic applications**

Dr. Oliviero Andreussi

University of North Texas



Dr. Andreussi earned his undergraduate degree (Italian Laurea, 5-years coursework) in Chemical Physics in 2003 from the University of Pisa and the Scuola Normale Superiore of Pisa. He earned a Ph.D. degree (2008) in Chemical Physics from Scuola Normale Superiore of Pisa. His Ph.D. research topic was on modeling the structure and dynamics of water at interfaces. He had several years of postdoctoral work, at MIT, Oxford, EPFL and the University of Pisa. In 2018, Dr. Andreussi began his appointment as an assistant professor at the Department of Physics of the University of North Texas, where he is currently doing research in computational physics of materials. More information about Dr. Andreussi and his research can be found at

<https://sites.google.com/site/olivieroandreussi/home> and at www.quantum-environ.org

Abstract

Continuum models of solvation have played a crucial role in the computational characterization of molecules solvated in neutral or electrolyte solutions. Recent advances in the field have extended the capabilities of this class of methods towards the characterization of solvated interfaces, possibly in the presence of an applied electrochemical potential. These recent advances have opened the possibility of modeling heterogeneous catalysis and electrochemistry in a first-principles-based framework, where the multiscale nature of the developed approaches provides a significant reduction of the computational burden while retaining a good accuracy. Here, the core methodological aspects and the most recent features of these recently developed approaches, as implemented in the ENVIRON library (www.quantum-environ.org), will be reviewed. Applications to the study of materials for electrocatalytic reactions will be presented, including a recent systematic screening of two-dimensional materials as electrocatalysts for the hydrogen evolution reaction (HER).